Table S1: Free Binding Energy scores of top 100 compounds

|  |  |  |
| --- | --- | --- |
| **Compound** | **Energy** | **VDW** |
| 100933831 | -180.2 | -180.2 |
| 159614 | -179.446 | -179.446 |
| 25006255 | -177.845 | -177.845 |
| 5388993 | -175.341 | -175.341 |
| 442111 | -175.207 | -175.207 |
| 56841098 | -174.732 | -174.732 |
| 74833942 | -174.446 | -174.446 |
| 5278403 | -173.048 | -173.048 |
| 44559284 | -172.609 | -172.609 |
| 45267183 | -172.579 | -172.579 |
| 11828754 | -169.194 | -169.194 |
| 154496988 | -168.062 | -168.062 |
| 6325522 | -165.655 | -165.655 |
| 5315216 | -164.003 | -164.003 |
| 100933832 | -163.59 | -163.59 |
| 56841094 | -162.433 | -162.433 |
| 124376 | -159.726 | -159.726 |
| 494490 | -158.871 | -158.871 |
| 42639328 | -158.476 | -158.476 |
| 102316658 | -157.57 | -157.57 |
| 24883980 | -156.664 | -156.664 |
| 198365 | -155.54 | -155.54 |
| 45358158 | -154.273 | -154.273 |
| 5320255 | -153.207 | -153.207 |
| 5315743 | -152.929 | -152.929 |
| 44559354 | -151.905 | -151.905 |
| 45267184 | -151.705 | -151.705 |
| 11767947 | -151.202 | -151.202 |
| 100925385 | -151.091 | -151.091 |
| 163188153 | -150.49 | -150.49 |
| 5315219 | -149.861 | -149.861 |
| 197026 | -149.694 | -149.694 |
| 5978 | -149.499 | -149.499 |
| 124516887 | -149.049 | -149.049 |
| 24188124 | -148.316 | -148.316 |
| 5315217 | -147.338 | -147.338 |
| 15575614 | -145.083 | -145.083 |
| 241903 | -144.839 | -144.839 |
| 163188151 | -144.79 | -144.79 |
| 5316490 | -143.33 | -143.33 |
| 5321583 | -142.966 | -142.966 |
| 3262516 | -142.567 | -142.567 |
| 21123523 | -142.439 | -142.439 |
| 5316334 | -141.877 | -141.877 |
| 5318981 | -141.597 | -141.597 |
| 442517 | -141.314 | -141.314 |
| 5315224 | -141.195 | -141.195 |
| 5748188 | -140.635 | -140.635 |
| 44559285 | -140.359 | -140.359 |
| 10919701 | -139.62 | -139.62 |
| 5315229 | -138.377 | -138.377 |
| 10128841 | -138.318 | -138.318 |
| 425978 | -135.201 | -135.201 |
| 261578 | -133.546 | -133.546 |
| 320745 | -133.539 | -133.539 |
| 42639327 | -133.349 | -133.349 |
| 14190180 | -133.174 | -133.174 |
| 2371 | -132.487 | -132.487 |
| 13342 | -131.693 | -131.693 |
| 163011235 | -130.179 | -130.179 |
| 162971130 | -130.119 | -130.119 |
| 162963996 | -129.2 | -129.2 |
| 163187317 | -129.14 | -129.14 |
| 3239 | -127.965 | -127.965 |
| 73197911 | -127.781 | -127.781 |
| 21304 | -126.65 | -126.65 |
| 42632433 | -126.505 | -126.505 |
| 5052 | -126.149 | -126.149 |
| 162947894 | -125.805 | -125.805 |
| 5315746 | -125.055 | -125.055 |
| 259898 | -124.9 | -124.9 |
| 5315221 | -124.875 | -124.875 |
| 11953924 | -123.789 | -123.789 |
| 13039027 | -123.608 | -123.608 |
| 5015264 | -122.549 | -122.549 |
| 156951 | -120.882 | -120.882 |
| 271304 | -119.522 | -119.522 |
| 5316748 | -118.109 | -118.109 |
| 86821 | -115.105 | -115.105 |
| 369002 | -114.961 | -114.961 |
| 98054312 | -113.045 | -113.045 |
| 22524494 | -112.909 | -112.909 |
| 269014 | -112.816 | -112.816 |
| 4485535 | -109.723 | -109.723 |
| 192740 | -107.483 | -107.483 |
| 3032566 | -107.373 | -107.373 |
| 5315215 | -104.594 | -104.594 |
| 601562 | -104.477 | -104.477 |
| 163083337 | -103.181 | -103.181 |
| 120879 | -103.084 | -103.084 |
| 12310173 | -102.229 | -102.229 |
| 162871248 | -102.197 | -102.197 |
| 163025450 | -98.5965 | -98.5965 |
| 162978917 | -97.7318 | -97.7318 |
| 163058109 | -97.5218 | -97.5218 |
| 5281243 | -97.0475 | -97.0475 |
| 45480560 | -96.9779 | -96.9779 |
| 161336 | -96.8786 | -96.8786 |
| 5321578 | -96.7055 | -96.7055 |
| 536803 | -95.5346 | -95.5346 |

Table S2: Bioactivity Scores of top 100 compounds.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Compound** | **GPCR ligand** | **Ion channel modulator** | **Kinase inhibitor** | **Nuclear receptor ligand** | **Protease inhibitor** | **Enzyme inhibitor** |
| 100933831 | -1.75 | -3.23 | -2.94 | -2.85 | -1.6 | -2.4 |
| 159614 | -3.3 | -3.64 | -3.66 | -3.58 | -3 | -3.52 |
| 25006255 | -1.03 | -2.05 | -1.59 | -1.53 | -0.68 | -1.16 |
| 5388993 | -2 | -3.13 | -3.17 | -2.94 | -1.68 | -2.55 |
| 442111 | -1.79 | -3.03 | -2.94 | -2.68 | -1.45 | -2.39 |
| 56841098 | -1.55 | -2.83 | -2.79 | -2.55 | -1.34 | -2.19 |
| 74833942 | -0.43 | -1.41 | -1.05 | -0.81 | -0.21 | -0.6 |
| 5278403 | -0.68 | -1.72 | -1.33 | -1.21 | -0.41 | -0.84 |
| 44559284 | -2.01 | -3.16 | -3.13 | -2.81 | -1.6 | -2.42 |
| 45267183 | -1.03 | -2.05 | -1.59 | -1.53 | -0.68 | -1.16 |
| 11828754 | -1.02 | -2.09 | -1.53 | -1.68 | -0.72 | -1.15 |
| 154496988 | -0.88 | -1.9 | -1.36 | -1.49 | -0.6 | -0.99 |
| 6325522 | -1.82 | -2.94 | -2.92 | -2.65 | -1.47 | -2.41 |
| 5315216 | -1.76 | -2.97 | -2.99 | -2.75 | -1.53 | -2.42 |
| 100933832 | -1.89 | -3.35 | -3.12 | -2.96 | -1.72 | -2.57 |
| 56841094 | -2.09 | -3.24 | -3.2 | -2.86 | -1.73 | -2.55 |
| 124376 | -2.03 | -3.23 | -3.23 | -2.91 | -1.64 | -2.57 |
| 494490 | -2.62 | -3.49 | -3.55 | -3.32 | -2.27 | -3.01 |
| 42639328 | -0.46 | -1.43 | -1.19 | -0.7 | -0.31 | -0.52 |
| 102316658 | -0.99 | -2.15 | -1.71 | -1.65 | -0.67 | -1.2 |
| 24883980 | -0.37 | -0.77 | -1.03 | -0.65 | -0.13 | -0.54 |
| 198365 | -1.88 | -3.02 | -3.05 | -2.64 | -1.53 | -2.45 |
| 45358158 | -2 | -3.13 | -3.17 | -2.94 | -1.68 | -2.55 |
| 5320255 | -1.39 | -2.47 | -2.33 | -1.85 | -0.98 | -1.66 |
| 5315743 | -2.01 | -3.21 | -3.13 | -2.88 | -1.64 | -2.62 |
| 44559354 | -2.01 | -3.21 | -3.13 | -2.88 | -1.64 | -2.62 |
| 45267184 | -0.56 | -1.6 | -1.22 | -1 | -0.29 | -0.76 |
| 11767947 | -1.56 | -2.88 | -2.77 | -2.57 | -1.29 | -2.22 |
| 100925385 | -1.76 | -2.97 | -2.99 | -2.75 | -1.53 | -2.42 |
| 163188153 | -1.79 | -3.03 | -2.94 | -2.68 | -1.45 | -2.39 |
| 5315219 | -1.88 | -3.02 | -3.05 | -2.64 | -1.53 | -2.45 |
| 197026 | -1.12 | -2.46 | -2.31 | -2.08 | -1.02 | -1.76 |
| 5978 | -2 | -3.13 | -3.17 | -2.94 | -1.68 | -2.55 |
| 124516887 | -1.76 | -2.97 | -2.99 | -2.75 | -1.53 | -2.42 |
| 24188124 | -0.53 | -1.24 | -1.5 | -1.61 | -0.73 | -0.97 |
| 5315217 | -2 | -3.09 | -3.13 | -2.9 | -1.68 | -2.58 |
| 15575614 | -1.12 | -2.46 | -2.31 | -2.08 | -1.02 | -1.76 |
| 241903 | -1.76 | -2.97 | -2.99 | -2.75 | -1.53 | -2.42 |
| 163188151 | -1.76 | -2.97 | -2.99 | -2.75 | -1.53 | -2.42 |
| 5316490 | 0.23 | 1.02 | -0.18 | 0.28 | 0.2 | 0.3 |
| 5321583 | 0 | -0.58 | -0.62 | 0.03 | 0.16 | 0.33 |
| 3262516 | 0.28 | 0.11 | -0.19 | -0.07 | 0.01 | 0.33 |
| 21123523 | -1.81 | -3.07 | -3 | -2.75 | -1.54 | -2.41 |
| 5316334 | -0.79 | -2.07 | -1.91 | -1.66 | -0.71 | -1.39 |
| 5318981 | -1.79 | -3.04 | -2.97 | -2.76 | -1.47 | -2.44 |
| 442517 | -0.73 | -1.46 | -1.34 | -1.1 | -0.41 | -0.94 |
| 5315224 | -2.01 | -3.15 | -3.16 | -2.96 | -1.69 | -2.59 |
| 5748188 | -0.88 | -1.89 | -1.35 | -1.42 | -0.59 | -0.97 |
| 44559285 | -1.8 | -3.01 | -2.92 | -2.6 | -1.59 | -2.41 |
| 10919701 | -0.88 | -1.9 | -1.36 | -1.49 | -0.6 | -0.99 |
| 5315229 | 0.41 | 0.23 | -0.12 | 0.41 | 0.23 | 0.25 |
| 10128841 | 0.05 | -0.17 | -0.09 | 0.32 | 0.01 | 0.18 |
| 425978 | 0.36 | 0.2 | -0.14 | 0.4 | 0.18 | 0.27 |
| 261578 | 0.42 | 0.27 | -0.12 | 0.44 | 0.24 | 0.32 |
| 320745 | -2.03 | -3.19 | -3.12 | -2.88 | -1.6 | -2.53 |
| 42639327 | -1.34 | -2.51 | -1.97 | -1.82 | -1 | -1.44 |
| 14190180 | -2.62 | -3.49 | -3.55 | -3.32 | -2.27 | -3.01 |
| 2371 | 0.31 | 0.03 | -0.5 | 0.93 | 0.14 | 0.55 |
| 13342 | -1.76 | -2.97 | -2.99 | -2.75 | -1.53 | -2.42 |
| 163011235 | -2.09 | -3.24 | -3.2 | -2.86 | -1.73 | -2.55 |
| 162971130 | 0.33 | 0.23 | -0.43 | -0.14 | 0 | 0.16 |
| 162963996 | 0.3 | 0.07 | -0.07 | 0.13 | 0.28 | 0.11 |
| 163187317 | -2 | -3.13 | -3.17 | -2.94 | -1.68 | -2.55 |
| 3239 | 0.2 | 0.08 | -0.28 | 0.57 | 0.28 | 0.48 |
| 73197911 | 0.26 | 0.19 | -0.17 | 0.78 | 0.32 | 0.61 |
| 21304 | 0.31 | 0.3 | -0.23 | 0.34 | 0.27 | 0.34 |
| 42632433 | -1.8 | -2.99 | -3.01 | -2.8 | -1.56 | -2.46 |
| 5052 | 0.1 | -0.36 | -0.39 | -0.36 | -0.02 | -0.21 |
| 162947894 | -1.02 | -2.09 | -1.53 | -1.68 | -0.72 | -1.15 |
| 5315746 | 0.5 | 0.29 | -0.1 | 0.5 | 0.3 | 0.34 |
| 259898 | -1.79 | -3.03 | -2.94 | -2.68 | -1.45 | -2.39 |
| 5315221 | 0.32 | -0.03 | -0.1 | 0.42 | 0.17 | 0.25 |
| 11953924 | -2.09 | -3.24 | -3.2 | -2.86 | -1.73 | -2.55 |
| 13039027 | 0.17 | 0.14 | -0.4 | 0.69 | 0.27 | 0.55 |
| 5015264 | 0.28 | 0.23 | -0.1 | -0.18 | 0.11 | 0.33 |
| 156951 | -1.81 | -3.07 | -3 | -2.75 | -1.54 | -2.41 |
| 271304 | 0.19 | -0.03 | -0.12 | 0.29 | 0.2 | 0.22 |
| 5316748 | 0.22 | 0.05 | -0.34 | 0.16 | 0.17 | -0.04 |
| 86821 | 0.14 | 0.04 | -0.51 | 0.73 | 0.07 | 0.51 |
| 369002 | 0.16 | 0.31 | -0.28 | 0.14 | 0.29 | 0.48 |
| 98054312 | 0.38 | 0.14 | -0.24 | 0.16 | 0.16 | 0.04 |
| 22524494 | 0.03 | -0.06 | -0.37 | -0.06 | 0.1 | 0.21 |
| 269014 | 0.14 | -0.09 | -0.13 | 0.25 | 0.13 | 0.17 |
| 4485535 | 0.11 | -0.01 | -0.18 | -0.29 | 0.03 | -0.09 |
| 192740 | 0.16 | -0.05 | -0.25 | -0.05 | 0.05 | 0.09 |
| 3032566 | 0.22 | -0.11 | -0.28 | 0.17 | 0.08 | 0.12 |
| 5315215 | -1.71 | -3.02 | -2.96 | -2.62 | -1.42 | -2.25 |
| 601562 | 0.28 | 0.1 | -0.25 | 0.14 | 0.13 | 0.47 |
| 163083337 | 0.33 | 0.09 | -0.22 | 0.23 | 0.27 | 0.15 |
| 120879 | 0.33 | 0.09 | -0.22 | 0.23 | 0.27 | 0.15 |
| 12310173 | 0.32 | 0.14 | -0.44 | 0.8 | 0.12 | 0.36 |
| 162871248 | 0.42 | 0.2 | -0.08 | -0.02 | 0.06 | 0.08 |
| 163025450 | -0.26 | -0.97 | -0.89 | -0.5 | -0.15 | -0.34 |
| 162978917 | 0.21 | 0.11 | -0.45 | 0.66 | 0.18 | 0.49 |
| 163058109 | 0.3 | 0.14 | -0.22 | 0.2 | 0.2 | 0.22 |
| 5281243 | 0.03 | -0.28 | -0.25 | 0.47 | -0.03 | 0.28 |
| 45480560 | 0.21 | 0.33 | -0.32 | 0.72 | 0.2 | 0.56 |
| 161336 | 0.28 | 0.11 | -0.19 | -0.07 | 0.01 | 0.33 |
| 5321578 | -0.27 | -0.91 | -0.43 | -0.59 | -0.19 | -0.17 |
| 536803 | 0.15 | 0.02 | -0.37 | 0.05 | -0.07 | 0.06 |